

Evidence of one-step replica symmetry breaking in a three-dimensional Potts glass model

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 (Dated: August 8, 2014)

We study a 7-state Potts glass model in three dimensions with first, second, and third neighbor interactions with a bimodal distribution of couplings by Monte Carlo simulations. Our results show the existence of a spin-glass transition at a finite temperature T_c , a discontinuous jump of an order parameter at T_c without latent heat, and a non-trivial structure of the order-parameter distribution below T_c . They are compatible with a one-step replica symmetry breaking.

PACS numbers: 05.10.Ln, 05.50.+q, 75.10.Nr, 75.40.Cx, 75.40.Mg

Introduction.— Mean-field spin-glass models without time reversal symmetry have been studied by many researchers over the last few decades. Being quite different from the Sherrington-Kirkpatrick Ising spin glass [1], a class of models such as p -spin model and p -state Potts glass model [2, 3], exhibit two distinct phase transitions [4, 5]. One is a dynamical phase transition at temperature T_d , below which exponentially large number of metastable states emerge and a spin autocorrelation function does not decay to zero in the long time limit. The latter is a consequence of the ergodicity breaking. The other is a purely thermodynamic transition at $T_c < T_d$, which is called “random first order transition” (RFOT). At T_c the entropy concerned with the metastable states vanishes and an order parameter emerges discontinuously without latent heat, and below T_c replica symmetry is broken at one-step level. A particularly intriguing fact is that at the mean-field level dynamical equations for a time correlation function near T_d in these models are formally identical to the mode-coupling equations in the theory of structural glass transition. This fact suggests a potentially deep connection between spin-glass models with quenched disorder and structural glasses with no quenched disorder. The whole of the phenomena described above is called RFOT scenario in the field of glass transition and is speculated to be a promising candidate for the mean-field description of the glass transition. Thus, the mean-field spin-glass theory has been developed in great detail, revealing that some spin-glass models are a prototypical model of the RFOT scenario at least at the mean-field level [5–7].

One of the main issues to be addressed is whether these mean-field predictions are valid in finite dimensions in which fluctuations must be taken into account. A straightforward way to investigate the effect of fluctuation is to examine finite dimensional spin-glass models which display RFOT in the mean-field limit. Previously, extensive Monte Carlo studies for the p -state Potts glass models in a three-dimensional cubic lattice clarified the existence of spin-glass transition at finite temperature for $p \leq 6$ [8–10]. However, their properties are rather com-

patible with those of continuous transition in the Ising spin-glass model and no clear remnants of RFOT have been found. In the mean-field theory, the discontinuity of the order parameter and also difference between T_d and T_c grow with the number of states in the p -state Potts glass model [11, 12]. Hence, it might be likely that RFOT, if any, could be found in the Potts glass models with relatively large p in finite dimensions. In addition, for such a large value of p , it is needed to make most of the couplings antiferromagnetic to prevent ferromagnetic ordering. On the other hand, as pointed out in Ref.[13], when most of the couplings are antiferromagnetic, the Potts glass models on any finite connectivity lattice are unfrustrated for large values of p in a sense that these couplings are easily satisfied in the ground state. Then, no glassy ordering is expected because the frustration is considered to be a key ingredient of the glassy behavior. Indeed, Brangian *et al.* found that there was no glassy phase in the 10-state Potts glass model with a bimodal distribution of the couplings with a small fraction of ferromagnetic couplings [14]. Thus, it is a difficult requirement to avoid the ferromagnetic ordering and to keep the frustration simultaneously for the Potts glass models with large p on finite connectivity lattices. In particular, in the three dimensional Potts glass model with only nearest-neighbor interactions, the low connectivity $c = 6$ makes it difficult to meet the requirement.

In order to avoid the above difficulties, we propose a Potts glass model with not only the nearest neighbor couplings, but also second- and third-nearest neighbor couplings on a three dimensional cubic lattice. Although this model has only short range interactions, such a high connectivity could yield the frustration even in the antiferromagnetic case and even for large p . Using Monte Carlo simulations for the p -state Potts glass model with $p = 7$, we obtained the following results: (1) This model shows a static spin-glass transition at finite temperature $T_c/J = 0.421(3)$ with the correlation length exponent $\nu = 0.68(9)$. (2) At T_c the order parameter appears discontinuously but no latent heat exists. (3) Below T_c the order-parameter distribution has a bimodal structure.

Model and Numerical Details. — The p -state Potts glass model we studied is defined by the Hamiltonian

$$\mathcal{H}_{\mathcal{J}}(\sigma) = - \sum_{(i,j)} J_{ij} \delta(\sigma_i, \sigma_j), \quad (1)$$

where the Potts spin σ_i on the site i takes $0, 1, \dots, p-1$ and the summation is over the nearest, second-nearest and third-nearest neighbors on a three-dimensional cubic lattice of size $N = L^3$ with periodic boundaries. Each of the sites has connectivity $c = 26$, and a set of coupling constants $\mathcal{J} = \{J_{ij}\}$ are quenched random variables chosen from a bimodal distribution $P(J_{ij}) = x\delta(J_{ij} - J) + (1-x)\delta(J_{ij} + J)$, where x denotes the fraction of ferromagnetic couplings. In order to prevent a ferromagnetic transition, we set $x = (1 - 1/\sqrt{2})/2 \simeq 0.15$ and $J = \sqrt{2}J_0$. Then, the mean and variance of the couplings are -1 and 1 , respectively, measured in the unit of J_0 . This means that most of the couplings are antiferromagnetic in this model. Note that because all the spins in the smallest cube with $L = 2$ interact with each other through up to the third-neighbor couplings, there remains the finite frustration for $p \leq 7$ even in the purely antiferromagnetic case. In this Letter, we focus on the case of $p = 7$.

Since spin-glass simulations are hampered by extremely slow relaxation dynamics, we use replica exchange Monte Carlo method [16]. The linear sizes are $L = 4 - 10$ for most of observables explained below and $L = 14$ for the energy density and the specific heat which are relatively easy to evaluate. The number of samples averaged over is $256 - 4096$ depending on the system size. The total number of Monte Carlo sweeps (MCS) used on

each lattice size is $10^6 - 10^8$. We examined equilibration by monitoring the Monte Carlo average of the observables while doubling the number of MCS for measurement successively. The data are regarded as equilibrium values when the last two data agree within their error bars.

Observables.— It is convenient to represent the Potts variables using the simplex representation [15], in which the spin variable \mathbf{S}_i of the site i takes one of p unit vectors $\{\mathbf{e}^{(\alpha)}\}_{\alpha=1}^p$ pointing to the corner of the simplex in the $p-1$ dimensional space. These vectors satisfy the relations $\mathbf{e}^{(\alpha)} \cdot \mathbf{e}^{(\beta)} = (p\delta_{\alpha,\beta} - 1)/(p-1)$. Some observables calculated in our simulations are expressed as those in vector spin glasses using the simplex representation. To study the spin-glass transition we define a spin-glass order parameter as an overlap between two replicas. For two independent replica configurations denoted as $\{\mathbf{S}_i^{(1)}\}_{i=1}^N$ and $\{\mathbf{S}_i^{(2)}\}_{i=1}^N$ with the same disorder, the wave-number dependent overlap between them for the Potts-glass model is defined by a tensor $q^{ab}(\mathbf{k})$:

$$q^{ab}(\mathbf{k}) = \frac{1}{N} \sum_{i=1}^N S_i^{a,(1)} S_i^{b,(2)} e^{i\mathbf{k} \cdot \mathbf{R}_i}, \quad (2)$$

where the upper suffixes a and b are indices of the simplex vector component and \mathbf{R}_i is a displacement vector at the site i . A rotational invariant scalar overlap is also defined by

$$q(\mathbf{k}) = \sqrt{\sum_{a,b}^{p-1} |q^{ab}(\mathbf{k})|^2}. \quad (3)$$

Then, the wave-number-dependent spin-glass susceptibility $\chi_{\text{SG}}(\mathbf{k})$ is given by an expectation value

$$\chi_{\text{SG}}(\mathbf{k}) = N \left[\langle q^2(\mathbf{k}) \rangle^{(T)} \right]_{\text{av}}, \quad (4)$$

where $[\dots]_{\text{av}}$ and $\langle \dots \rangle^{(T)}$ represent an average over the quenched disorder and a thermal average at temperature T , respectively. The dimensionless correlation length ξ_L/L is useful for estimating the critical temperature T_c because it is independent of L at T_c . Thus, the intersection temperature in the plot of ξ_L/L for various L gives the estimate of T_c . The finite-size correlation length ξ_L is estimated from $\chi_{\text{SG}}(\mathbf{k})$ as [17]

$$\xi_L = \frac{1}{2 \sin(|\mathbf{k}_{\min}|/2)} \sqrt{\frac{\chi_{\text{SG}}(\mathbf{0})}{\chi_{\text{SG}}(\mathbf{k}_{\min})} - 1}, \quad (5)$$

where $\mathbf{k}_{\min} = (2\pi/L, 0, 0)$ is the smallest nonzero wave vector. Another dimensionless quantity is the Binder parameter defined by

$$g_4 = \frac{(p-1)^2}{2} \left(1 + \frac{2}{(p-1)^2} - \frac{[\langle q^4(\mathbf{0}) \rangle^{(T)}]_{\text{av}}}{[\langle q^2(\mathbf{0}) \rangle^{(T)}]_{\text{av}}^2} \right). \quad (6)$$

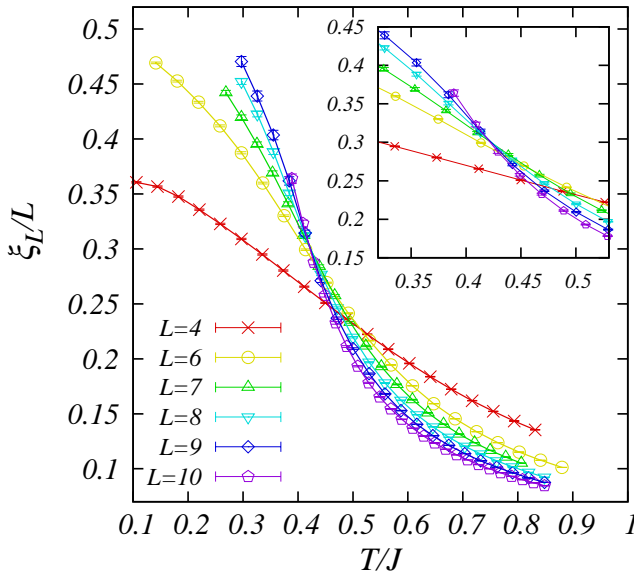


FIG. 1. (Color Online) Temperature dependence of the dimensionless correlation length ξ_L/L . The inset shows its enlarged view around the transition temperature.

This quantity is known to exhibit a peculiar behavior for systems with a one-step RSB (1RSB) transition [18–20], while it is expected to exhibit the intersection at a conventional second order transition temperature.

One of the most important quantities for studying the phase space structure of the spin-glass phase is the overlap distribution function

$$P^{(T)}(Q) = \left[\langle \delta(Q - q(\mathbf{0})) \rangle^{(T)} \right]_{\text{av}}, \quad (7)$$

which is accessible from Monte Carlo simulations. The overlap distribution function has a non-trivial structure if the replica symmetry breaking occurs. In particular, two separated peaks appear in $P^{(T)}(Q)$ at and below T_c for a 1RSB system, that is similar to the order-parameter distribution found in systems with a first-order transition.

Numerical results.— First, in order to investigate critical properties of the Potts glass model, we see the finite-size correlation length ξ_L scaled by L . As shown in Fig. 1, a clear intersection is observed around $T/J \simeq 0.4$, though it is slightly shifted to low temperature with increasing L . The intersection for asymptotically large L provides an evidence of spin-glass phase transition at the temperature. The Potts glass model for $p = 7$ with nearest neighbor interactions has no glassy phase at up to very low temperature, possibly down to zero with the present fraction of ferromagnetic couplings. The second- and third-neighbor couplings cause the spin-glass transition temperature to increase significantly. To determine T_c and ν , we perform a finite-size scaling analysis in which

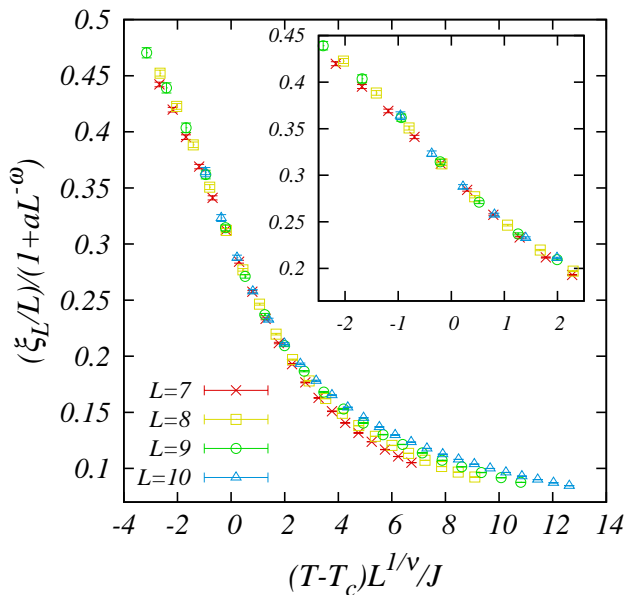


FIG. 2. (Color Online) Scaling plot of the finite-size correlation length ratio ξ_L/L according to Eq.(8) using $T_c/J = 0.421$, $\nu = 0.68$, $a = 1$ and $\omega = 3$. The inset shows its magnified view.

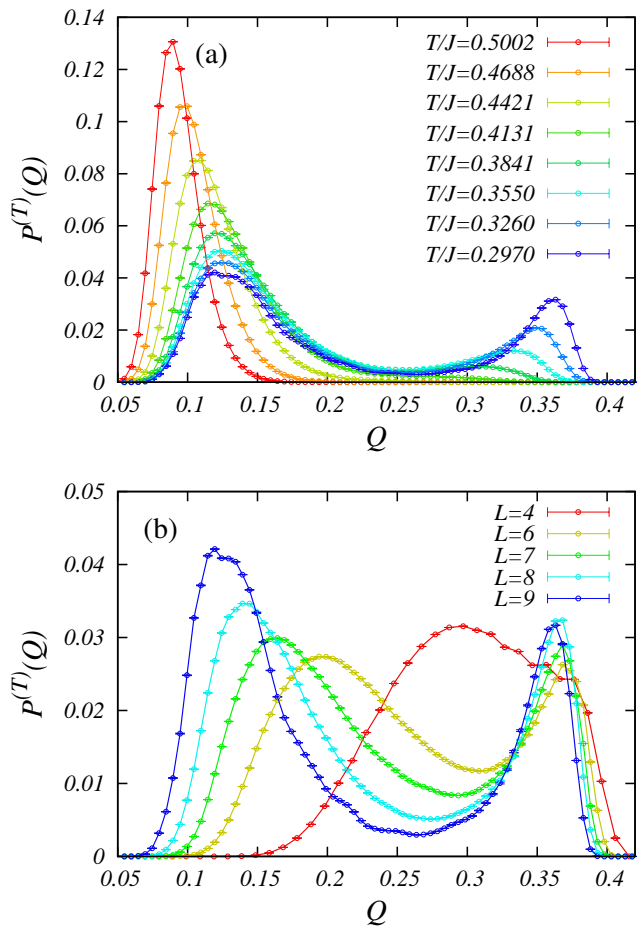


FIG. 3. (Color Online) Overlap distribution function of a Potts glass model in three dimensions for various temperatures with $L = 9$ (a) and for different sizes at $T/J = 0.2970$ below T_c (b).

the dimensionless correlation length is assumed to follow the scaling form, up to the leading correction term,

$$\frac{\xi_L}{L} = \tilde{X} \left((T - T_c) L^{1/\nu} \right) (1 + aL^{-\omega}), \quad (8)$$

where ν is the correlation length exponent, ω is an exponent of the leading correction, and \tilde{X} is an universal scaling function. The scaling parameters such as T_c and ν are determined by requiring all the curves of $\xi_L / (L(1 + aL^{-\omega}))$ against $(T - T_c)L^{1/\nu}$ to collapse on a single curve near T_c . Bayesian scaling analysis recently developed [22] is used to perform the scaling analysis systematically. Fig.2 shows the scaling plot of ξ_L/L , which is obtained by

$$T_c/J = 0.421(3), \quad \nu = 0.68(9). \quad (9)$$

The value of ν is consistent with $2/d$ where d is the spatial dimension, derived by a heuristic scaling argument based on RFOT [21], suggesting that the overlap function has a finite jump at T_c . This is in contrast with the

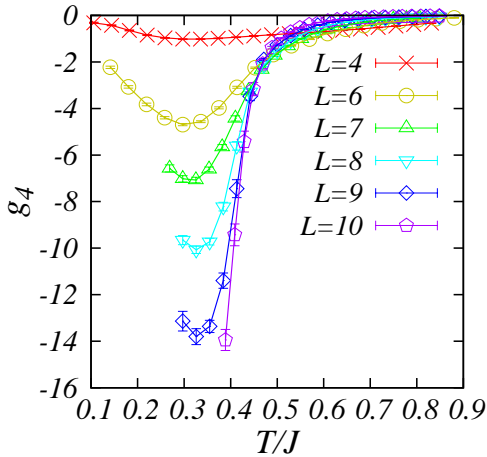


FIG. 4. (Color Online) Temperature dependence of the Binder parameter g_4 of a Potts glass model in three dimensions.

fact that the value of ν is slightly larger than $2/d$ in the three-dimensional Potts-glass models with the nearest-neighbor couplings [8–10].

In Fig. 3, temperature and system-size dependence of $P^{(T)}(Q)$ is shown. At high temperatures the distribution function has a single Gaussian-like peak near $Q \simeq 0$. The peak position is expected to approach zero in the thermodynamic limit. On the other hand, below T_c another peak at a larger value of Q , corresponding to the Edwards-Anderson order parameter q_{EA} , emerges and coexists with the other peak at lower Q . The lower panel in Fig. 3 shows the size dependence of $P^{(T)}(Q)$ at $T/J = 0.2970$, which is well below the estimated T_c . The peaks at $Q = q_{EA}$ and $Q \simeq 0$ show a tendency to grow in height and become narrower in width with increasing L . Further, the weight between these two peaks is strongly suppressed with L . These imply that the bimodal structure in $P^{(T)}(Q)$ remains in the thermodynamic limit, providing a clear evidence of the 1RSB nature in the spin-glass phase.

While Fig. 3(a) suggests that the overlap emerges discontinuously at T_c , the peak of $P^{(T)}(Q)$ near T_c is rounded by the finite-size effect. Another evidence of the discontinuous jump is found, however, in temperature dependence of the Binder parameter g_4 . As shown in Fig. 4, g_4 exhibits a negative dip near T_c with a negatively divergent tendency for large L . Note that $g_4 \rightarrow -\infty$ at T_c when a 1RSB transition with a finite jump of q_{EA} occurs in the mean-field glass models [18, 20], in contrast to a continuous full RSB transition and also an ordinary second order phase transition. Thus, this divergent behavior implies that q_{EA} appears at T_c discontinuously.

Finally, Fig. 5 shows temperature dependence of the energy density and the specific heat. No discontinuity of the energy density, and hence no divergent tendency in the specific heat are observed at around T_c . Instead, the

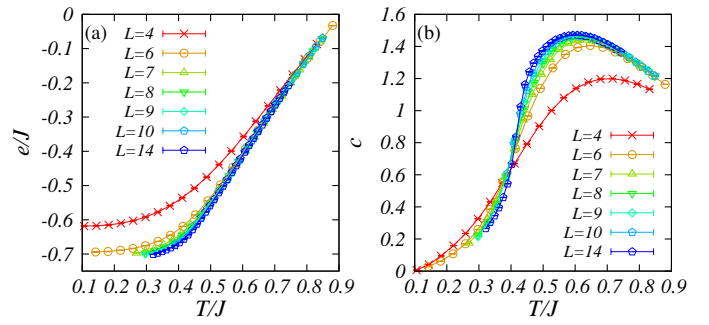


FIG. 5. (Color Online) Temperature dependence of the energy density (a) and the specific heat (b) of a Potts glass model in three dimensions.

specific heat for various sizes has an intersection near T_c . This might indicate that in the thermodynamic limit the specific heat has a discontinuous jump at T_c as expected from some mean-field spin-glass models with RFOT. Further study is required to clarify this point.

Conclusions.— In this letter, the 7-state Potts glass model with the nearest, second-nearest and third-nearest neighbor interactions has been proposed as a candidate for displaying RFOT in finite dimensions. A key ingredient is to keep both a large number of Potts states and the frustration. All of our equilibrium numerical results suggest that the present model in three dimensions shares many features of RFOT, namely a spin-glass transition at finite temperature, a jump of the spin-glass order parameter at T_c without latent heat, and a bimodal overlap distribution below T_c , as expected from 1RSB. Thus, we conclude that this is the first realization of the finite-dimensional statistical-mechanical model which mimics a static part of the whole RFOT scenario. Another important aspect of the RFOT scenario is dynamical properties, which are believed to be modified in finite dimensions from the mean-field predictions. This model provides a promising test bed for further examining the validity of the RFOT scenario in finite dimensions, which remains to be investigated.

The authors thank S. Sasa for useful discussions. The authors also thank S. Takabe and Y. Nishikawa for carefully reading the manuscript. Numerical simulation in this letter has mainly been performed by using the facility of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This research was supported by the Grants-in-Aid for Scientific Research from the JSPS, Japan (Nos. 22340109, 25120010 and 25610102), and JSPS Core-to-Core program “Nonequilibrium dynamics of soft matter and information.”

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